HIGH-PERFORMANCE SIMULATION OF SURFACE-SUBSURFACE COUPLED FLOW AND REACTIVE TRANSPORT AT WATERSHED SCALE

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Abstract

It is forecasted that two out of three persons in the world will be water stressed by the year of 2025 (EPA 1998). Proper management of water resources at watershed scale may offer the best solutions for water shortage and contamination. The objective of the research is to conduct reactive flow simulations in surface-subsurface, coupled flow systems using a high-performance version of WASH123D. WASH123D is a watershed hydrology simulator that utilizes the method of characteristics to solve land surface fluid dynamic equations and the Galerkin finite element method to solve subsurface groundwater flow equations. A Lagrangian-Eulerian finite element method is used to solve the reactive solute transport equations. Parallelisms of the high-performance WASH123D are implemented in MPI (Message Passing Interface) by using the parallel library PETSc. The goal is to evaluate the practicality of applying WASH123D to large realistic problems and to identify additional steps towards parallelism optimization. Initial results on high-performance platforms are encouraging in speeding up calculations of a real-world problem.

Keywords: Watershed, Reactive Flow, Finite Element, High-Performance Computing.

Introduction

Watershed hydrology models such as HSPF (Hydrological Simulation Program Fortran, Bicknell et al., 1997) have been widely used to study the movement of water and pollutants through various hydrological regimes. Though HSPF and similar watershed hydrology models are process based, their treatment of the transport and transformation of water and pollutants in various hydrological regimes are not explicit and mechanistic. This report presents a next generation watershed hydrology model, WASH123D (Yeh et al., 1998), and demonstrates its application to flow and pollutant transport problems, in

the context of parallel, high-performance computing. In WASH123D, the mass and momentum balance equations are explicitly solved in both overland and subsurface flow regimes. The objective of this research is to improve the performance of the WASH123D simulator, in particular, by implementing MPI (Message Passing Interface) parallelisms in the simulator on massively parallel, high-performance computers.

Method

The Hydrological Simulator WASH123D

The hydrological simulator WASH123D is a multidimensional, Lagrangian-Eulerian, finite element, hydrology model that solves the universal mass and energy balance equations. WASH123D may be used to simulate the transfer of heat and the transport of mass including water, sediment, and dissolved and adsorbed species in watershed systems. Flow of water in river networks and on ground surface is modeled by one of the following approaches - kinematic, diffusive, or dynamic wave, depending on the slope of the ground surface. Subsurface flow of water is described by the Richards equation that accounts for water flow through variably saturated porous media. Surface and subsurface flow of water are tightly coupled in WASH123D. In solving the overland flow equations, WASH123D employs the backward method of characteristics (MOC) or the Lagrangian approach. The Galerkin finite element method is used to solve the Richard's equation.

Parallelism Implementation

The following parallelisms are implemented in the WASH123D sequential code to improve its performance on massively parallel computers:

1. The one-, two- and three-dimensional finite element meshes of the land surface and the subsurface models of WASH123D are first divided in a consistent manner into subdomains by using the mesh partitioning software modules provided by METIS and ParMETIS (e.g., see Schloegel, Karypis and Kumar, 2000). The subdomains are then distributed to the processors of a parallel computer.
2. In solving the linearized equations as results of applying the Galerkin finite element method, we use the linear and nonlinear parallel solver PETSc (http://www-unix.mcs.anl.gov/petsc/petsc-2/). The work of assembling the mass matrices is distributed as suggested above as equally as possible to the individual processes with the aims of minimizing message passing overhead and balancing the computational loads.
3. The computation of backward particle at the finite element nodes is distributed to the parallel processors cyclically. The solution of chemical transformation on one finite element node is essentially independent of that on another. This step is followed by a global gather-scatter operation to collect newly obtained results, in particular, for subsequent Eulerian step of the chemical transport calculation.

Result and Discussion

Reactive Transport Simulation

Because of various land use practices, waterways may be polluted by agricultural chemicals absorbed in the soil matrix. Shown in Figure 1 is an example that demonstrates the leaching of agricultural chemicals from a farm on one side of a river reach. The chemicals are initially applied only to the land
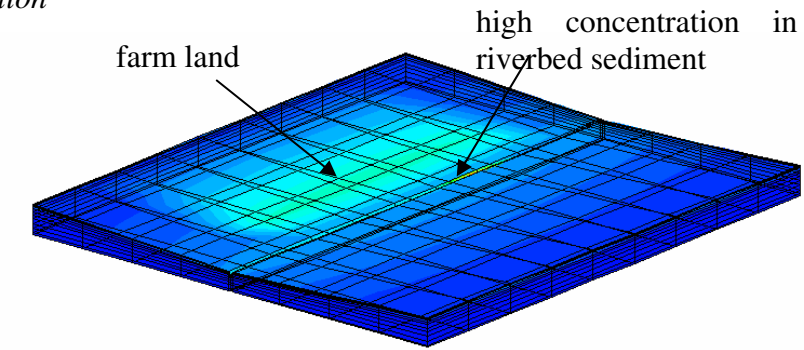

Figure 1. Coupled model simulation of the transport of agricultural chemicals from soil matrix of a farm land. The contour shows chemical concentrations in the solid phase.

surface in solid form. Because of their high concentrations in the soil matrix, the continuous leaching of the chemicals results in high concentrations in the riverbed sediment. The chemicals washed into the river and those desorbed from riverbed sediments eventually may affect water quality of not only the upstream area near the farm land but also downstream areas, posing a water quality problem at a scale much larger than the farm land itself.

Parallel Performance

The parallelisms implemented in WASH123D are tested against a real-world application of the Dade County watershed in southern Florida, USA. Shown in Figure 2 is the simulation domain of the watershed with calculated
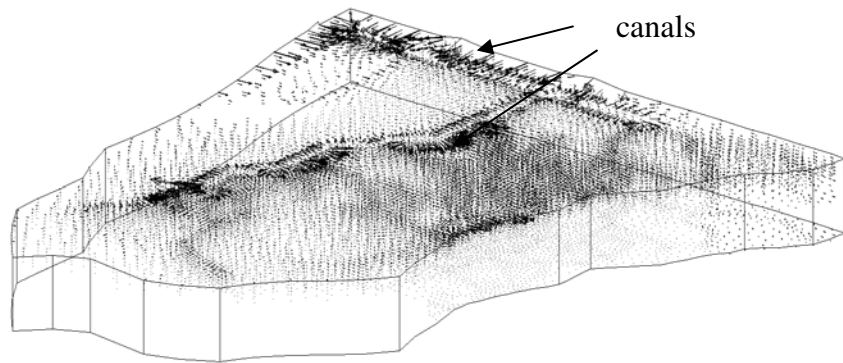

Figure 2. Groundwater velocity vectors calculated by WASH123D for the Dade County Watershed.

groundwater flow velocity vectors. The simulation domain was divided into multiple subdomains, ranging from 2 to 64 with corresponding number of processors, in the simulations. The calculation includes only the flow regimes in the canals, the land surface, and the subsurface. The performance test is conducted on the 184-node IBM RS/6000 SP (Eagle) operated by the Computer Science and Mathematics Division of Oak Ridge National Laboratory. The performance results are shown in Figure 3.
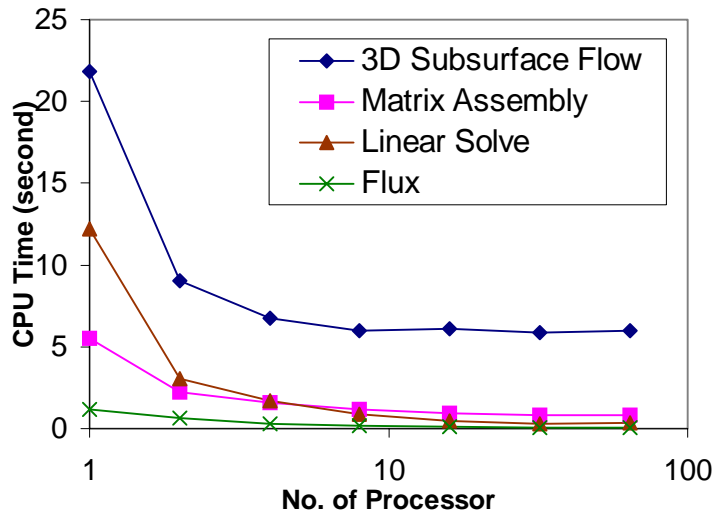
Figure 3. Parallel performance on an IBM RS/6000 SP using a 37,760 finite element node problem.

The velocity vector plot in Figure 2 clearly indicates the effect of the canals on the subsurface, as groundwater sinks and sources at various locations of the watershed. The parallel performance test suggests that, for the Dade County model with 37,760 finite element nodes, the parallelism scales relatively well up to 8 processors. The overall speed-up of the flow calculation levels off with higher number of processors. However, the performance of the linear matrix solver and the flux calculation continues to improve as the number of processors increases. These indicate that the performance may improve only if the size of the problem is increased with the number of processors. Nonethelesss, for the intermediate size problem of the Dade County watershed, the parallel performance is encouraging and may largely improve the efficiency of large field scale studies.

Acknowledgement

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